

Computations of Multivalued Solutions in Nonlinear PDEs

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Problems Interested

We are interested in the numerical computations of **multivalued** solutions that appear in many physical problems

- high frequency (dispersive) wave propagations
- geometric optics, semiclassical limits of (non)linear Schrödinger equations
- multiple arrivals in tomography and seismic migration
- electron beam modulation in vacuum electronic devices
- multilane traffic flow modeling
- queueing system, supply chains

These physical problems are described by non-linear PDEs (hyperbolic, Hamilton-Jacobi, etc.) that admit singularities (caustics, weak breaking, etc.). Classical *viscosity solution* fails to give the physically correct solutions.

A Survey of Numerical Approaches

- kinetic equations in phase space
- moment equations
- level set method

A Physical Example: The Schrodinger Equations

Consider the linear and nonlinear Schrödinger equations in the **semiclassical** regimes

$$i\epsilon \psi_t + \frac{\epsilon^2}{2} \Delta \psi - V\psi = 0 \quad \mathbf{x} \in R^d, \quad t > 0$$
$$\psi(\mathbf{x}, 0) = A_0(\mathbf{x}) e^{i \frac{S_0(\mathbf{x})}{\epsilon}}$$

In this equation, $\psi(\mathbf{x}, t)$ is the complex-valued *wave function*, ϵ is or is playing the role of *Planck's constant*. It is assumed to be small here. The solution ψ and the related physical observables become *oscillatory* in space and time in the order of $O(\epsilon)$, causing all the mathematical and numerical challenges.

Numerical Issues

Such a problem is an excellent example of **multi-scale** problems, with one scale at the quantum ($O(\epsilon)$) scale and the other one at the scale of classical mechanics which governs the evolution of the envelope equation.

Because of the small scale $O(\epsilon)$, typically, a direct numerical solution of the (linear) Schrödinger equation requires

- For finite difference schemes (Leap-Frog, Dufort-Frankel, Crank-Nicolson, etc.), the mesh sizes and time steps need to be $o(\epsilon)$ in order to get the correct physical observables. This result is *sharp*. (**Markowich, Pietra, Pohl, Stimming, 1999 & 2001**)

- The meshing strategy will improve to $O(\epsilon)$ (for linear problem the time step will be independent of $O(\epsilon)$) if a *time-splitting spectral method* is used. (**Bao-Jin-Markowich, 2002**)
- One basically has to numerically **resolve** the small scale of $O(\epsilon)$. In multi-D such a constraint is a severe numerical burden

Semiclassical Limit of Schrödinger equations

If one can find the asymptotic (semiclassical) limit as $\epsilon \rightarrow 0$ then one can just solve the *limiting* equation numerically. In this way the meshing strategy becomes ϵ -independent. This might be possible for *linear* problems (of course at this level the quantum information is lost and one is solving the *classical mechanics*—which has many interests in its own right).

A classical way to study the semiclassical limit is the **WKB** method. We assume that solution has the form (*Madelung Transform*)

$$\psi(\mathbf{x}, t) = A(\mathbf{x}, t)e^{i\frac{S(\mathbf{x}, t)}{\epsilon}}$$

and apply this *ansatz* into the Schrödinger equation with initial data. Separating the real part from the imaginary part, and keeping only the leading order term, one can get

$$S_t + \frac{1}{2}|\nabla S|^2 + V = 0 \quad \text{eiconal equation}$$

$$(|A|^2)_t + \nabla \cdot (|A|^2 \nabla S) = 0 \quad \text{transport equation}$$

This limit can be justified for smooth solutions (**Grenier 98**). Beyond the singularity (*caustics*) of the eiconal equation this system is no longer the correct *weak solution* of the semiclassical limit of the Schrödinger equations, even for linear problem. For example, in the linear case, the Schrödinger equation satisfies the **superposition principle**, while the *viscosity* solution, in the sense of **Crandall and Lions**, for the eiconal equation beyond the caustics, is **not** linearly superimposable.

Quantum Hydrodynamics Equations

If one applies the Madelung Transformation to the Schrödinger equations *without* dropping higher order terms, one gets

$$\begin{aligned} (|A|^2)_t + \nabla \cdot (|A|^2 \nabla S) &= 0, \\ (|A|^2 \nabla S)_t + \nabla \cdot [|A|^2 \nabla S \otimes \nabla S] + |A|^2 \nabla V \\ &= \frac{\epsilon^2}{2} |A|^2 \nabla \left(\frac{1}{|A|} \Delta |A| \right). \end{aligned}$$

This is a system of pressureless or isentropic gas equations with a **dispersive** correction. Beyond shock or caustic the solution becomes oscillatory. The *zero dispersive limit* is a rather subtle mathematical issue (**Lax-Levermore theory for KdV**).

Clearly *viscosity solution* is inappropriate here.

Semiclassical Limit in the Phase Space

A convenient tool to study the semiclassical limit is the **Wigner transformation**

$$W^\epsilon(\mathbf{x}, \mathbf{k}) = \left(\frac{1}{2\pi}\right)^d \int_{R^d} e^{i\mathbf{k}\cdot\mathbf{y}} \psi\left(\mathbf{x} - \frac{\mathbf{y}}{2}\right) \bar{\psi}\left(\mathbf{x} + \frac{\mathbf{y}}{2}\right) d\mathbf{y}$$

where $\bar{\psi}$ is the complex conjugate of ψ . (**Lions-Paul; Gèrard, Markowich, Mauser, Poupaud**)

The connection between W and ψ is established through the moments

$$\begin{aligned} \int_{R^d} W^\epsilon(\mathbf{x}, \mathbf{k}) d\mathbf{k} &= |\psi(\mathbf{x})|^2 \\ \int_{R^d} \mathbf{k} W^\epsilon(\mathbf{x}, \mathbf{k}) d\mathbf{k} &= \frac{1}{2i} (\psi \nabla \bar{\psi} - \bar{\psi} \nabla \psi) \\ \int_{R^d} |\mathbf{k}|^2 W^\epsilon(\mathbf{x}, \mathbf{k}) d\mathbf{k} &= |\nabla \phi(\mathbf{x})|^2 \end{aligned}$$

The Wigner equation

As $\epsilon \rightarrow 0$, the limit Wigner equation is the **Liouville equation** in phase space

$$W_t + \mathbf{k} \cdot \nabla_{\mathbf{x}} W - \nabla V \cdot \nabla_{\mathbf{k}} W = 0$$

with the initial condition

$$W(0, \mathbf{x}, \mathbf{k}) = |A_0(\mathbf{x})|^2 \delta(\mathbf{k} - \nabla S_0(\mathbf{x}))$$

The semiclassical limit for moments

For smooth solution, the solution

$$\psi(\mathbf{x}, t) = A(\mathbf{x}, t) e^{i \frac{S(\mathbf{x}, t)}{\epsilon}}$$

has a limit

$$W(t, \mathbf{x}, \mathbf{k}) = |A(t, \mathbf{x})|^2 \delta(\mathbf{k} - \nabla S(t, \mathbf{x}))$$

Applying this ansatz to the Liouville equation one gets the *eiconal* equation for the phase S and *transport* equation for amplitude $|A|^2$, recovering the result by WKB.

Let

$$\begin{aligned} \rho(t, \mathbf{x}) &= |A(t, \mathbf{x})|^2 \\ \rho(t, \mathbf{x}) \mathbf{u}(t, \mathbf{x}) &= \rho(t, \mathbf{x}) \nabla S(t, \mathbf{x}) \end{aligned}$$

Then these “fluid variables” satisfy the *pressureless* gas dynamics equations

$$\begin{aligned} \rho_t + \nabla \cdot (\rho \mathbf{u}) &= 0, \\ (\rho \mathbf{u})_t + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) + \rho \nabla V &= 0, \end{aligned}$$

Kinetic Moment Closure

Since the Liouville equation is a *kinetic* equation defined in the *phase* space (**six dimensional !**), it is too expensive to solve numerically. We hope to bring it down to the physical space. This usually requires special density distribution (**Grad, Levermore**).

We are interested in computing the **multivalued** or **multiphase** solutions. If the total number of phases is **finite**, we can find a limiting distribution for W^ϵ that can be used to close the Liouville equations **exactly**

Multiphase Ansatz

Use the **stationary phase method** or the **Fourier integral operators**, one can prove that, if the total number of phases is $N < \infty$, then

$$\psi \approx \sum_{k=1}^{N(\mathbf{x},t)} \psi_k(\mathbf{x},t) = \sum_{k=1}^{N(\mathbf{x},t)} A_k(\mathbf{x},t) e^{i\frac{S_k(\mathbf{x},t)}{\epsilon}}.$$

In addition, we have $\mathbf{u}_k(\mathbf{x},t) = \nabla S_k(\mathbf{x},t) \neq \mathbf{u}_j(\mathbf{x},t)$ for $k \neq j$ and A_k 's are bounded away from 0.

If one calculates the Wigner function, one can find its limit to be (away from the caustics)

$$w(\mathbf{x}, \mathbf{v}, t) = \sum_{k=1}^{N(\mathbf{x},t)} \rho_k \delta(\mathbf{v} - \mathbf{u}_k)$$

Moreover, each (ρ_k, \mathbf{u}_k) satisfies the pressureless gas equations.

Sparber, Markowich, Mauser;

Jin-Xiantao Li

Moment equations in 1-D

Define the moments

$$m_l = \int_R w(x, v, t) v^l dv, \quad l = 0, 1, \dots, 2N.$$

In addition, we define the density and velocity by

$$\rho(x, t) = m_0, \quad u(x, t) = \frac{m_1}{m_0}.$$

Multiplying the Liouville equation in 1-d by v^l , $l = 0, 1, \dots, 2N - 1$ and integrating over v , one obtains the moment equations in the physical space

$$\partial_t m_0 + \partial_x m_1 = 0,$$

$$\partial_t m_1 + \partial_x m_2 = -m_0 \partial_x V,$$

.....

$$\partial_t m_{2N-1} + \partial_x m_{2N} = -(2N - 1) m_{2N-2} \partial_x V.$$

Moment Closure in 1-D

With the multiphase ansatz, one has

$$m_l = \sum_{k=1}^N \rho_k u_k^l, \quad l = 0, 1, \dots, 2N.$$

With these one can close the moment system by expressing m_{2N} as a function of m_0, \dots, m_{2N-1} ,

$$m_{2N} = F_N(m_0, m_1, \dots, m_{2N-1}),$$

provided the $2N \times 2N$ system

$$m_l = \sum_{k=1}^N \rho_k u_k^l, \quad l = 0, 1, \dots, 2N - 1$$

is invertible, allowing us to express $(\rho_k, u_k, k = 1, \dots, N)$ in terms of $m_0, m_1, \dots, m_{2N-1}$. If this is true, the function F_N can be defined and consequently the multiphase equations are equivalent to the N pressureless gas equations satisfied by each (ρ_k, u_k) (thus the moment systems are *weakly hyperbolic*—the Jacobian is similar to Jordan blocks).

Two-Phase equations in 1-D

If $N = 2$, then one obtains four moment equations

$$\begin{aligned}\partial_t m_0 + \partial_x m_1 &= 0, \\ \partial_t m_1 + \partial_x m_2 &= -m_0 \partial_x V, \\ \partial_t m_2 + \partial_x m_3 &= -2m_1 \partial_x V, \\ \partial_t m_3 + \partial_x m_4 &= -3m_2 \partial_x V,\end{aligned}$$

with

$$m_4 = \frac{m_3^2 m_0 - 2m_1 m_2 m_3 + m_2^3}{m_0 m_2 - m_1^2}.$$

Clearly, m_4 is not well-defined if $\frac{m_0 m_2 - m_1^2}{\rho_1 \rho_2} = (u_2 - u_1)^2 = 0$ (when there is just *one* phase). We modify m_4 as follows:

$$m_4 = \begin{cases} \frac{m_3^2 m_0 - 2m_1 m_2 m_3 + m_2^3}{m_0 m_2 - m_1^2}, & \text{if } m_0 m_2 - m_1^2 \neq 0; \\ \frac{m_2^2}{m_0}, & \text{Otherwise.} \end{cases}$$

Then the moment system is good for both single and double phases, whichever emerges.

Phase boundaries are **undercompressive shocks**

Higher Moment Equations

Similar moment equations can be obtained for larger N (algebraically the flux becomes increasingly more complicated with larger N and one needs to use numerical procedure to generate the flux F_N for $N > 5$).

F_N is always a rational function of m_0, \dots, M_{2N-1} , and the zero denominator condition can be used to determine the correct number of phases as was done for $N = 2$. Similar modified flux may also be introduced.

We have also found moment equations for 2-D.

One can estimate the total number of phases in 1-D (number of initial inflection points). For multi-D physical intuition is needed for such an estimate.

The Work of Brenier and Corrias ('98)

It was observed by **Brenier '84** that the geometric solution to

$$\partial_t u + u \partial_x u = 0, \quad u(x, 0) = u^0 \geq 0$$

is given exactly by

$$\partial_t f + \xi \partial_x f = 0, \quad f(0, x, \xi) = H(u^0(x) - \xi) H(\xi)$$

where H stands for the Heaviside function. After folds develop in finite time, f becomes

$$f(t, x, \xi) = \sum_{k=1}^{N(t)} (-1)^{k-1} H(u_k(t, x) - \xi), \quad u_k > u_{k+1}$$

This function is selected according to an *entropy minimization principle*, which makes it possible to close a moment system of K equations by expressing the $K + 1^{st}$ moment in terms of the K moments preceding it under the constraint of satisfying some entropy condition.

When $K = 1$ this is the kinetic formulation for entropy solution of the Burger's equation by **Lions-Perthame-Tadmor '94**.

Engquist and Runborg '96 used this idea to compute multiphase geometrical optics from the *wave equation*.

Relationship between BC's and Our Moment Systems:(Gosse-Jin-Li 02)

- If the number of phases is **correct**, the moment systems are the **same**. If the number of phases is not enough, they differ (different ways to introduce artificial shocks). This justifies that BC's system, if enough number of phases is used, *is the correct semiclassical limit for the linear Schrödinger equation*
- BC's idea is restricted to 1-D. The Wigner approach gives a general formulation of moment systems in **any dimension**

A Kinetic Scheme for Moment Systems

Since the moment system is only *weakly* hyperbolic, and the flux function cannot be expressed analytically when N is large, the *Godunov* type scheme is out of the question. On the other hand, it arises as a moment closure of the kinetic Liouville equation, thus a kinetic scheme is the most natural choice for the moment systems.

Euler-Poisson Systems for Klystron

joint work with X. Li, J. Wöhlbier and J. Booske

- Vacuum electronics devices for high power, high frequency electromagnetic waves sources and amplifiers
- The source of energy for amplification is a high energy beam of electrons that interact with an electromagnetic wave at input cavity, causing electron beam velocity modulation to obtain electron beam current modulation, which is converted into amplified electromagnetic radiation at the output cavity
- For strong enough input RF "driver", some electrons are sped up sufficiently such that they **pass by**, or "**overtaking**" other slower electrons. In Eulerian description, a *multi-valued* velocity function is needed to describe such overtaking phenomenon

put the Klystron figure here

The Governing equations – the Euler Poission equations

$$\begin{aligned}\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial z}(\rho u) &= 0 \\ \frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial z}(\rho u^2) &= R\rho E \\ \frac{\partial}{\partial z}E &= \rho - 1\end{aligned}$$

with boundary conditions

$$\begin{aligned}\rho(z = 0, t) &= 1, \\ u(z = 0, t) &= 1 + 1/2 \sum_n \epsilon_n \sin(\omega_n T t + \theta_n)\end{aligned}$$

A Kinetic Approach

We go to the phase space and write down the Vlasov-Poisson system

$$\begin{aligned}w_t + vw_z + RE(z, t)w_v &= 0 \\E_z &= \int_{R^+} w(z, v, t) dv - 1 \\(z, v, t) &\in R \times R^+ \times R^+, \end{aligned}$$

with the boundary value

$$w(0, v, t) = \rho^0(t)\delta(v - u^0(t))$$

Define the moments

$$\rho = \int_{R^+} w(z, v, t) dv \quad I = \rho u = \int_{R^+} w(z, v, t)v dv$$

One can argue that if the bicharacteristics are smooth (*no mathematical proof yet*), and $v > 0$, then the multi-phase solution is valid:

$$w(z, v, t) = \sum_{k=1}^N \rho_k \delta(v - u_k)$$

and one can use it to close the V-P equations and obtain system of moment equations.

A kinetic scheme can be introduced to solve the moment system.

A Level Set Approach

- Liouville equation based level set approach was already used by *Osher etc, Fomel and Sethian* to compute **fronts** of eiconal equations, namely the bicharacteristics.
- There has been no such approach that can compute the solution in the **entire** physical domain.
- joint work with **S. Osher**
- independent work of Liu-Cheng-Osher

A Level Set Method for Quasilinear Hyperbolic Equations

Based on a mathematical formulation in *Courant-Hilbert*.

We consider Let $u(t, \mathbf{x}) \in \mathfrak{R}$ be a scalar satisfying an initial value problem of an d -dimensional first order hyperbolic PDE with source term:

$$(1) \quad \partial_t u + \mathbf{F}(u) \cdot \nabla_{\mathbf{x}} u + q(\mathbf{x}) = 0,$$

$$(2) \quad u(0, \mathbf{x}) = u_0(\mathbf{x}).$$

Here $\mathbf{F}(u) : \mathfrak{R}^d \rightarrow \mathfrak{R}^d$ is a vector, and $q : \mathfrak{R}^d \rightarrow \mathfrak{R}$ is the source term. We introduce a level set function $\phi(t, \mathbf{x}, p)$ in dimension $d + 1$, whose zero level set is the solution u :

$$(3) \quad \phi(t, \mathbf{x}, p) = 0 \quad \text{at} \quad p = u(t, \mathbf{x}).$$

Therefore we evolve the entire solution u as the zero level set of ϕ .

The Level Set Equation

One can easily show that the level set function satisfies a simple linear hyperbolic equation in R^{d+1} :

$$(4) \quad \partial_t \phi + \mathbf{F}(p) \cdot \nabla_{\mathbf{x}} \phi - q(\mathbf{x}) \partial_p \phi = 0.$$

The initial condition for ϕ can be chosen simply as

$$(5) \quad \phi(0, \mathbf{x}, p) = p - u_0(\mathbf{x}).$$

if $u_0(\mathbf{x})$ is continuous, or as the *signed distance function* if $u_0(\mathbf{x})$ is discontinuous (so ϕ is always continuous).

Multidimensional Hamilton-Jacobi equations

Consider the time dependent, d -dimensional Hamilton-Jacobi equation

$$(6) \quad \partial_t S + H(\mathbf{x}, \nabla_{\mathbf{x}} S) = 0,$$

$$(7) \quad S(0, \mathbf{x}) = S_0(\mathbf{x}).$$

Introduce $\mathbf{u} = (u_1, \dots, u_d) = \nabla_{\mathbf{x}} S$. Taking the gradient on the H-J equation, one gets an equivalent (at least for smooth solutions) form of the Hamilton-Jacobi equation

$$(8) \quad \partial_t \mathbf{u} + \nabla_{\mathbf{x}} H(\mathbf{x}, \mathbf{u}) = 0,$$

$$(9) \quad \mathbf{u}(0, \mathbf{x}) \equiv \mathbf{u}_0(\mathbf{x}) = \nabla_{\mathbf{x}} S_0(\mathbf{x}).$$

About the Conservation Law Formulation

This conservation law formulation was used by *Jin-Xin* ('99) to construct numerical schemes for the original Hamilton-Jacobi equation. A key condition to guarantee the condition is that \mathbf{u} *remains a gradient*:

$$(10) \quad \mathbf{u} = \nabla_{\mathbf{x}} S ,$$

which ensures that

$$(11) \quad \nabla_{\mathbf{x}} \mathbf{u} = \nabla_{\mathbf{x}}^2 S$$

is the Hessian matrix of S thus is *symmetric*, namely,

$$(12) \quad (\nabla_{\mathbf{x}} \mathbf{u})^T = \nabla_{\mathbf{x}} \mathbf{u} .$$

This is a critical condition for our derivation of the level set equation.

Level Set Equation for H-J

We use d level set functions $\phi_i = \phi_i(t, \mathbf{x}, \mathbf{p})$, $i = 1, \dots, d$, where $\mathbf{p} = (p_1, \dots, p_d) \in \mathbb{R}^d$, such that the intersection of their zero level sets yields \mathbf{u} , namely,

$$\phi_i(t, \mathbf{x}, \mathbf{p}) = 0 \quad \text{at} \quad \mathbf{p} = \mathbf{u}(t, \mathbf{x}), \quad i = 1, \dots, d \quad (13)$$

Then one can show that ϕ_i satisfies

$$(14) \quad \partial_t \phi + \nabla_{\mathbf{p}} H \cdot \nabla_{\mathbf{x}} \phi - \nabla_{\mathbf{x}} H \cdot \nabla_{\mathbf{p}} \phi = 0.$$

It is the Liouville equation, which is linear hyperbolic with variable coefficients since in (14) $H = H(\mathbf{x}, \mathbf{p})$.

A convenient initial condition for each ϕ_i , $i = 1, \dots, n$ can be taken as:

$$(15) \quad \phi_i(0, \mathbf{x}, \mathbf{p}) = p_i - u_i(\mathbf{x}).$$

One should use the signed distance function if the initial data are discontinuous.

Local level set method can be used to reduce the cost to $O(N^d \ln N)$

Computing density and other physical observables

If one is interested in also computing the density, or other physical observables (momentum, energy, etc.), the solving directly the continuity equation

$$\rho_t + \nabla \cdot \rho \mathbf{u} = 0$$

will be difficult when \mathbf{u} is multivalued.

One can of course solve the Liouville equation

$$W_t + \mathbf{k} \cdot \nabla_{\mathbf{x}} W - \nabla V \cdot \nabla_{\mathbf{k}} W = 0$$

with the measure-valued initial data

$$W(0, \mathbf{x}, \mathbf{k}) = |A_0(\mathbf{x})|^2 \delta(\mathbf{k} - \nabla S_0(\mathbf{x}))$$

This involves 1) approximating the delta function initially and then 2) numerically evolving a "delta" function in time.

Due to numerical dissipation the accuracy will be low.

Phase space computation of physical observables (S. Jin, H.L. Liu, S. Osher and R. Tsai)

We now consider the following two problems.

$$\begin{aligned}\partial_t f + \mathbf{k} \cdot \nabla_{\mathbf{x}} f - \nabla V \cdot \nabla_{\mathbf{k}} f &= 0, \\ f(0, \mathbf{x}, \mathbf{k}) &= \rho_0(\mathbf{x});\end{aligned}$$

$$\begin{aligned}\partial_t \phi + \mathbf{k} \cdot \nabla_{\mathbf{x}} \phi - \nabla V \cdot \nabla_{\mathbf{k}} \phi &= 0, \\ \phi(0, \mathbf{x}, \mathbf{k}) &= \mathbf{k} - \mathbf{u}_0(\mathbf{x}).\end{aligned}$$

we can prove that

$$(16) \quad W(t, \mathbf{x}, \mathbf{k}) = f(t, \mathbf{x}, \mathbf{k}) \delta(\phi(t, \mathbf{x}, \mathbf{k})).$$

The physical observables of the Liouville equation are thus given by

$$\begin{aligned}\bar{\rho} &= \int W d\mathbf{k} = \int f(t, \mathbf{x}, \mathbf{k}) \delta(\phi(t, \mathbf{x}, \mathbf{k})) d\mathbf{k}, \\ \bar{\rho \mathbf{u}} &= \int \mathbf{k} W d\mathbf{k} = \int \mathbf{k} f(t, \mathbf{x}, \mathbf{k}) \delta(\phi(t, \mathbf{x}, \mathbf{k})) d\mathbf{k}.\end{aligned}$$

We only evaluating the delta function numerical at the end (postprocessing)!

Conclusions

We presented several different approaches for highly oscillatory and multi-valued solutions that arise in a wide variety of applications: geometric optics, semiclassical Schrödinger, modulated electron beam in vacuum electronic devices, dispersive waves, seismic waves, multilane traffic flows, queueing systems ...

- *Kinetic approach*– for more general class of physical problems, including the Euler-Poisson, and has more information throughout moments, but needs to deal with measured-value solutions
- *moment approach* – cost minimum, but complicated in high phases or dimensions
- *level set method* – more accurate than kinetic approach, can use developed tools (such as local level set method) in level set methods, yet to make it work for nonlinear systems

- Still many challenging questions: theoretic justifications, computations of undercompressive shocks, discontinuous fluxes, multi-d, ...